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Methylcyclohexane

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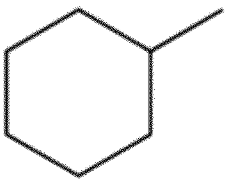
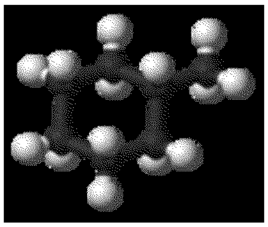
Methylcyclohexane





IUPAC name

methylcyclohexane

Other names

Hexahydrotoluene
Cyclohexylmethane
Toluene hexahydride

Identifiers	
CAS number	108-87-2
PubChem	7962
ChemSpider	7674
Jmol-3D images	Image 1

SMILES

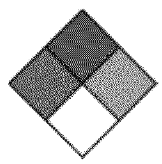
- CC1CCCCC1

InChI

- InChI=1S/C7H14/c1-7-5-3-2-4-6-7/h7H,2-6H2,1H3

Key: UAEPNZWRGJTJPN-UHFFFAOYSA-N ✓Y

InChI=1/C7H14/c1-7-5-3-2-4-6-7/h7H,2-6H2,1H3
Key: UAEPNZWRGJTJPN-UHFFFAOYAG

Properties	
Molecular formula	C_7H_{14}
Molar mass	98.19 g mol^{-1}
Appearance	Colourless liquid
Density	0.77 g/cm^3
Melting point	−126.3 °C; −195.3 °F; 146.8 K
Boiling point	101 °C; 214 °F; 374 K
Solubility in water	Insoluble in water
Hazards	
Main hazards	severe fire hazard
NFPA 704	 3 1 0
Flash point	−3 °C; 27 °F; 270 K

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Infobox references

Except where noted otherwise, data are given for materials in their standard state (at 25 °C (77 °F), 100 kPa)

Methylcyclohexane is a colourless liquid with a faint benzene-like odour. Its molecular formula is C_7H_{14}. Methylcyclohexane is used in organic synthesis and as a solvent for cellulose ethers. It is a component of jet fuel and is also a component of correction fluids.

Contents

Structure[edit]

Monosubstituted methylcyclohexane has one methyl branch on one carbon of the cyclohexane ring. Like all substituted cyclohexanes, it can ring-flip rapidly between two chair conformations.

However, a monosubstituted Methylcyclohexane exists almost exclusively in the equatorial position rather than axial. When the methyl group occupies the axial position, there is steric crowding (steric strain) by the axial hydrogens on the same side of the ring (known as the 1,3-diaxial interactions). There are two such interactions, with each methyl/hydrogen pair contributing approximately 7.61 kJ/mol strain. However, the equatorial conformation experiences no such interaction so it is more stable.

Disubstituted cyclohexanes[edit]

Main article: Cyclohexane conformation

Cyclohexanes could also have more than one methyl branch. **Disubstituted** cyclohexane, or also known as **dimethylcyclohexane** has two methyl branches. Unlike the monosubstituted cyclohexane, there are several possible structures. The methyl groups could be on the same carbon, separate carbons and it doesn't necessarily have to be on the same face. The 1,3-diaxial strain interactions still apply to the disubstituted. If the methyl groups are on different faces and both in axial positions, there are diaxial interactions with the axial hydrogen groups on both faces. If they are on the same face, both methyl groups interact with the one hydrogen that is in axial position and there is also a methyl-methyl interaction with a steric energy of approximately 15.3 kJ/mol. If the methyl groups are on adjacent carbons of the cyclohexane, with one of them axial and the other equatorial, there would be a gauche interaction which adds to the total strain energy the molecule has. For the dimethylcyclohexane which has two methyl groups on one carbon (1,1-dimethylcyclohexane), one methyl group is axial and the other equatorial. It would have the same total strain energy as the monosubstituted cyclohexane with axial methyl.

Jet Fuel Surrogates[edit]

Methylcyclohexane is one of a group of fuels that have recently been used as components for jet fuel surrogate blends.[1] Chemical analysis of Jet A finds a high cycloparaffin content; methylcyclohexane is one of the hydrocarbons used as Jet A surrogate in order to mimic this high presence of cycloparaffin and the associated chemical behaviour of the fuel.

References[edit]

This article **needs additional citations for verification**. Please help improve this article by adding citations to reliable sources. Unsourced material may be challenged and removed. *(November 2011)*

1. ^ Ji, C.; Egolfopoulos, F.N. (2011). "Hydrogen Flame propagation of mixtures of air with binary liquid fuel mixtures". *Proc. Comb. Inst.* **33**: 955–961. doi:10.1016/j.proci.2010.06.085. Cite uses deprecated parameters (help)

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